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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant : Bemis et al.
Serial No. : 10/781,015
Filed : February 17, 2004
Title : MOLECULAR MODELING METHODS

Art Unit : 1631
Examiner : Unknown

MAIL STOP AMENDMENT
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Copies of the references listed on the attached form PTO-1449 are enclosed.

This statement is being filed before the receipt of a first Office Action on the merits.

Please apply any charges or credits to Deposit Account No. 06-1050, referencing attorney docket number 14435-003001.

Respectfully submitted,

Date: 3-10-05

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Substitute Form PTO-1449 (Modified)	U.S. Department of Commerce Patent and Trademark Office	Attorney's Docket No. 14435-003001	Application No. 10/781,015
Information Disclosure Statement by Applicant (Use several sheets if necessary) (37 CFR §1.98(b))		Applicant Bemis et al.	
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U.S. Patent Documents

Examiner Initial	Desig. ID	Document Number	Publication Date	Patentee	Class	Subclass	Filing Date If Appropriate
	AA						
	AB						

Foreign Patent Documents or Published Foreign Patent Applications

Examiner Initial	Desig. ID	Document Number	Publication Date	Country or Patent Office	Class	Subclass	Translation Yes	Translation No
	AC							
	AD							

Other Documents (include Author, Title, Date, and Place of Publication)

Examiner Initial	Desig. ID	Document
	AE	Allen "The Cambridge Structural Database: a quarter of a million crystal structures and rising" *Acta. Cryst.* B58:380-388 (2002)
	AF	Bemis et al. "A fast and efficient method for 2D and 3D molecular shape description" *J. Comp-Aided Mol. Des.* 6:607-628 (1992)
	AG	Berman et al. "The Nucleic Acid Database, A Comprehensive relational database of three-dimensional structures of nucleic acids" *Biophys. J.* 63:751-759 (1992)
	AH	Berman et al. "The Protein Data Bank" *Nuc. Acids. Res.* 28(1):235-242 (2000)
	AI	Böhm et al. "The computer program LUDI: A new method for the de novo design of enzyme inhibitors" *J. Comput-Aided Mol. Des.* 6:61-78 (1992)
	AJ	Brooks et al. "CHARMM: A Program for Macromolecular Energy, Minimization, and Dynamics Calculations" *J. Comput. Chem.* 4:187-217 (1983)
	AK	Charifson et al. "Consensus Scoring: A Method for Obtaining Improved Hit Rates from Docking Databases of Three-Dimensional Structures into Proteins" *J. Med. Chem.* 42:5100-5109 (1999)
	AL	Eldridge et al. "Empirical scoring functions: I. The development of a fast empirical scoring function to estimate the binding affinity of ligands in receptor complexes" *J. Comput-Aided Mol. Des.* 11:425-445 (1997)
	AM	Flower "SERF: A program for accessible surface area calculations" *J. Mol. Graphics Model.* 15:238-244 (1998)
	AN	Gasteiger et al. "Chemical Information in 3D Space" *J. Chem. Inf. Comput. Sci.* 36:1030-1037 (1996)
	AO	Gasteiger et al. "Automatic Generation of 3D-Atomic Coordinates for Organic Molecules" *Tetrahed Comp. Meth.* 3:537-547 (1990)
	AP	Gehlhaar et al. "Molecular recognition of the inhibitor AG-1343 by HIV-1 protease: conformationally flexible docking by evolutionary programming" *Chem. Bio.* 2:317-324 (1995)
	AQ	Guex et al. "SWISS-MODEL and the Swiss-PdbViewer: An environment for comparative protein modeling" *Electrophoresis* 18:2714-2723 (1997)
	AR	Halgren "Merck Molecular Force Field. I. Basis, Form, Scope, Parameterization, and Performance of MMFF94" *J. Comput. Chem.* 17:490-519 (1996)

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	AS	Halgren "Merck Molecular Force Filed. II. MMFF94 van der Waals and Electrostatic Parameters for Intermolecular Interactions" *J. Comput. Chem.*17:520-552 (1996)
	AT	Halgren "Merck Molecular Force Field. III. Molecular Geometries and Vibrational Frequencies for MMFF94" *J. Comput. Chem* 17:553-586 (1996)
	AU	Holm et al. "Protein Structure Comparison by Alignment of Distance Matrices" *Mol. Biol.* 233:123-138 (1993)
	AV	Jones et al. "Development and Validation of a Genetic Algorithm for Flexible Docking" *J. Mol. Biol.* 267(3):727-748 (1997)
	AW	Jorgensen et al. "Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids" *J. Am. Chem. Soc.* 118:11225 (1996)
	AX	Kleywegt et al. "Detecting Folding Motifs and Similarities in Protein Structures" *Meth. Enzymol.* 277:525-545 (1997)
	AY	Lemmen et al. "Computational methods for the structural alignment of molecules" *J. Comp-Aided Molec. Des.*14:215-232 (2000)
	AZ	Madej et al. "Threading a Database of Protein Cores" *Proteins* 23:356-369 (1995)
	AAA	McLachlan "Rapid comparison of protein structures" *Acta. Cryst.* A38:871-873 (1982)
	ABB	Meng et al. "Automated Docking with Grid-Based Energy Evaluation" *J. Comp. Chem.* 13:505-524 (1992)
	ACC	Miller et al. "FLOG: A system to select 'quasi-flexible' ligands complementary to a receptor of known three dimensional structure" *J. Comput-Aided Mol. Des.* 8:153-174 (1994)
	ADD	Murray et al. "Empirical scoring functions. II. The testing of an empirical scoring function for the prediction of ligand-receptor binding affinities and the use of Bayesian regression to improve the quality of the model" *J. Comput-Aided Mol. Design* 12:503-519 (1998)
	AEE	Murtagh et al. "A Survey of Recent Advances in Hierarchical Clustering Algorithms" *The Computer J.* 26:354-359 (1983)
	AFF	Murzin et al. "SCOP: A Structural Classification of Proteins Database for the Investigation of Sequences and Structures" *J. Mol. Biol.* 247:536-540 (1995)
	AGG	Nilakantan et al. "Topological Torsion: A New Molecular Descriptor for SAR Applications. Comparison with Other Descriptors" *J. Chem. Inf. Comput. Sci.* 27:82-85 (1987)
	AHH	Nissink et al. "A New Test Set for Validating Predictions of Protein-Ligand Interaction" *Proteins* 49:457-471 (2002)
	AII	Pierce et al. "Kinase Inhibitors and the Case for CH···O Hydrogen Bonds in Protein-Ligand Binding" *Proteins* 49:576 (2002)
	AJJ	Russell "Detection of Protein Three-dimensional Side-chain Patterns: New Examples of Convergent Evolution" *J. Mol. Biol.* 279:1211-1227 (1998)
	AKK	Sadowski et al. "From Atoms and Bonds to Three-Dimensional Atomic Coordinates: Automatic Model Builders" *Chem. Rev.* 93:2567-2581 (1993)
	ALL	Schmitt et al. "A New Method to Detect Related Function Among Proteins Independent of Sequence and Fold Homology" *J. Mol. Biol.* 323:387-406 (2002)
	AMM	Shindyalov et al. "Protein structure alignment by incremental combinatorial extension (CE) of the optimal path" *Protein Engin.* 11(9):739-747 (1998)
	ANN	Shoichet et al. "Molecular Docking Using Shape Descriptors" *J. Comput. Chem.* 13:380-397 (1992)

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	AOO	Stouch et al. "A Simple Method for the Representation, Quantification, and Comparison of the Volumes and Shapes of Chemical Compounds" *J. Chem. Inf. Comput. Sci.* 26:4-12 (1986)
	APP	Walters et al. "Prediction of 'drug-likeness'" *Adv. Drug Deliv. Rev.* 54(3):255-271 (2002)
	AQQ	Walters et al. "Recognizing molecules with drug-like properties" *Curr. Opin. Chem. Biol.* 3(4):384-387 (1999)
	ARR	Walters et al. "Virtual screening – an overview" *Drug. Disc. Today* 3:160-178 (1998)
	ASS	

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